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Evidence for a metallic–like state in the T = 0 K phase diagram of a high temperature superconductor

A.A. Schmidt[1], J.J. Rodríguez-Núñez[2], and I. Ţifrea[3,a]

[1] Departamento de Matemática, CCNE, Universidade Federal de Santa Maria, 97105-900 Santa Maria, RS, Brazil
[2] Departamento de Física–FACYT, Universidad de Carabobo, Valencia 2001, Edo. Carabobo, Venezuela
[3] Department of Physics and Astronomy, University of Iowa, Iowa City, IA 52242, USA
 and Department of Theoretical Physics, University of Cluj, Cluj 3400, Romania

Abstract. We examine the effects of a phenomenological pseudogap on the $T = 0$ K phase diagram of a high temperature superconductor within a self-consistent model which exhibits a d-wave pairing symmetry. At the mean-field level the presence of a pseudogap in the normal phase of the high temperature superconductor is proved to be essential for the existence of a metallic–like state in the density versus interaction phase diagram. In the small density limit, at high attractive interaction, bosonic–like degrees of freedom are likely to emerge. Our result should be relevant for underdoped high temperature superconductors, where there is a strong evidence for the presence of a pseudogap in the excitation spectrum of the normal state quasiparticles.

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1 Introduction

One of the latest addition to the already very reach phase diagram of high temperature superconductors (HTSC) is represented by the so called pseudogap line ($T = T^*$). However, such a line is not well defined, and it should be understood more as a boundary limit which divides HTSC's temperature–density phase diagram into two distinct regions [1]. At temperatures $T_c < T < T^*$ (T_c represents the critical temperature for the normal–superconducting phase transition) and low doping, HTSC display a gap in the energy spectrum of the single-particle excitations associated to the normal state. Usually addressed as the *pseudogap*, this anomalous property of HTSC was originally seen in direct measurements of the single particle excitation spectra in angle resolved photoemission spectroscopy (ARPES) [2] and tunneling experiments [3]. The origin of the pseudogap in HTSC above the transition critical temperature T_c is not clear, as it is not clear its connection to the superconductivity phenomena. However, the symmetry of the pseudogap follows the superconducting gap symmetry and is of d-wave type [2]. The characteristic temperature T^* decreases with increasing the doping, eventually intersecting the $T = 0$ line at a *universal* critical point [4]. The existence of such a

critical point in the cuprates phase diagram is still under debate, different approaches relying on the fact that the T^* line merges with the T_c line at a doping value of the order of the optimal doping, where the transition temperature T_c has its maximum [1]. Different authors [5–7] suggest that the pseudogap and superconductivity in HTSC have the same cause, the idea of preformed pairs being of main importance to these theories. Other theories relate the pseudogap to antiferromagnetic fluctuations [8], spin-charge separation [9], or incommensurate charge–density–wave instabilities [10].

Experimental data for both normal and superconducting state in HTSC prove that standard theories such as the Fermi liquid theory of metals and BCS theory of superconductivity fail to correctly describe the physics of these materials. Such a behavior is attributed to the fact that correlations in HTSC are much stronger than in standard superconductors. In particular, the small coherence length of the Cooper pairs measured in HTSC (typically about 10–20 Å) suggested that HTSC belong to a class of compounds which can be viewed in a crossover regime between BCS superconductivity and Bose-Einstein condensation (BEC). From the theoretical point of view, the possibility of a crossover interpolation between BCS and BEC behavior was suggested previous to the HTSC discovery by Eagles [12] and latter on developed by Leggett [13], and

Noziéres and Schmitt–Rink [14]. More recently, various authors [15] discussed the HTSC phase diagram in terms of a BCS–BEC crossover, with the main conclusion that at least for the underdoped region of the phase diagram a BEC–like description is more appropriate to account for their unusual properties. On the other hand one should mention that ARPES data prove that below T^* the pseudogap opens only around the M points in the Brillouin zone, other regions of the Fermi surface being gapless. To account for such a behavior, one should consider a model with strong correlations around the M points and a weak interaction for the rest of the Brillouin zone, in other words to consider a two–gap model with a strong anisotropy [11].

Here we investigate the effects of the pseudogap on the $T = 0$ K HTSC phase diagram. We choose to treat the pseudogap at the phenomenological level in order to understand its influence on the physical properties of the superconducting state in HTSC. We consider that both the pseudogap and the superconducting gap are of d-wave symmetry and we neglect effects related to the anisotropy. First we will analyze the role and the effects of the pseudogap in the weak coupling limit, based on a modified BCS-like model. The main result will be that the presence of the pseudogap induces a critical value for the attractive electron–electron interaction responsible for the formation of a superconducting phase. Secondly, we extend this model to the strong interaction limit, using an approach similar to the crossover interpolation between BCS-like superconductivity and BEC. In this limit we will prove the existence of a metallic-like region in the phase diagram oh cuprates, a region induced by the pseudogap presence.

2 The model

The presence of the pseudogap in the energy spectrum of the normal state electrons in HTSC materials will strongly influence their physical properties not only in the normal state but also in the superconducting state. To account for such a change, we will treat the pseudogap at a phenomenological level. Accordingly, we consider that the normal state can be described by a modified one-particle Green's function which includes effects related to the pseudogap presence [16],

$$G^{-1}\left(\vec{k}, \omega\right) = \omega + \mu - \epsilon\left(\vec{k}\right) - \Sigma\left(\vec{k}, \omega\right), \qquad (1)$$

where ω represents the frequency and μ the chemical potential. For the case of two–dimensional (2D) structures the electronic energy dispersion is given by $\epsilon(\vec{k}) = -2t[\cos(k_x) + \cos(k_y)] + 4t\alpha'\cos(k_x)\cos(k_y)$, where nearest–, and next–nearest–neighbor interactions are included. The effects related to the pseudogap presence are introduced in the self-energy, which we consider to be

$$\Sigma\left(\vec{k}, \omega\right) = -E_g^2 \phi^2\left(\vec{k}\right) G_0\left(\vec{k}, \omega\right), \qquad (2)$$

where E_g is a constant, $\phi(\vec{k}) = \cos(k_x) - \cos(k_y)$ is related to the d-wave pseudogap symmetry, and $G_0(\vec{k}, \omega)$ is the free electron Green's function. A similar form of the electronic self-energy was used by Randeria [5] to explain the ARPES experimental results. We assume that such a form of the self–energy will be valid regardless the value of the coupling between the constituent electrons. The $T = 0$ K mean-field equation describing the superconducting state for the case of a fully separable attractive interaction in the presence of the pseudogap is obtained following the standard procedure [17]

$$\frac{1}{V} = \frac{1}{\pi^2}\int_0^\pi dk_x \int_0^\pi dk_y \frac{\phi^2\left(\vec{k}\right)\left[\psi^+\left(\vec{k}\right) - \psi^-\left(\vec{k}\right)\right]}{2\Delta_0\sqrt{\Delta_0^2 + 4E_g^2}}, \quad (3)$$

where

$$\psi^\pm(\vec{k}) = \frac{A_0^\pm}{\sqrt{\left[\epsilon\left(\vec{k}\right) - \mu\right]^2 + A_0^\pm \phi^2\left(\vec{k}\right)}}, \qquad (4)$$

$$A_0^\pm = E_g^2 + \frac{1}{2}\left[\Delta_0^2 \pm \Delta_0\sqrt{\Delta_0^2 + 4E_g^2}\right], \qquad (5)$$

and Δ_0 represents the superconducting gap. In the absence of the pseudogap ($E_g = 0$) equation (3) reduces to the standard BCS form. To include effects beyond the weak coupling limit, along with equation (3) we consider also the $T = 0$ K density equation

$$\rho = \frac{1}{\pi^2}\int_0^\pi dk_x \int_0^\pi dk_y \left[\alpha_2\left(\vec{k}\right) + \alpha_4\left(\vec{k}\right)\right], \qquad (6)$$

where

$$\alpha_2\left(\vec{k}\right) =$$
$$\frac{-\left[\omega_+^2\left(\vec{k}\right) - \left(\epsilon\left(\vec{k}\right) - \mu\right)^2\right] G^{-1}\left(\vec{k}, -\omega_2\left(\vec{k}\right)\right)}{\left[\omega_2\left(\vec{k}\right) - \omega_1\left(\vec{k}\right)\right]\left[\omega_2\left(\vec{k}\right) - \omega_3\left(\vec{k}\right)\right]\left[\omega_2\left(\vec{k}\right) - \omega_4\left(\vec{k}\right)\right]},$$

$$\alpha_4\left(\vec{k}\right) =$$
$$\frac{-\left[\omega_-^2\left(\vec{k}\right) - \left(\epsilon\left(\vec{k}\right) - \mu\right)^2\right] G^{-1}\left(\vec{k}, -\omega_4\left(\vec{k}\right)\right)}{\left[\omega_4\left(\vec{k}\right) - \omega_1\left(\vec{k}\right)\right]\left[\omega_4\left(\vec{k}\right) - \omega_2\left(\vec{k}\right)\right]\left[\omega_4\left(\vec{k}\right) - \omega_3\left(\vec{k}\right)\right]},$$

with

$$\omega_\pm^2\left(\vec{k}\right) = \left[\epsilon\left(\vec{k}\right) - \mu\right]^2 + \left[\Delta_0^2/2 + A_0^\pm\right]\phi^2\left(\vec{k}\right),$$

$\omega_1(\vec{k}) = |\omega_+(\vec{k})|$, $\omega_2(\vec{k}) = -|\omega_+(\vec{k})|$, $\omega_3(\vec{k}) = |\omega_-(\vec{k})|$, and $\omega_4(\vec{k}) = -|\omega_-(\vec{k})|$. The two self-consistent equations (3) and (6) will be solved together to include the strong interaction effects on the chemical potential, a procedure which will allow us to interpolate between weak and strong coupling limits.

3 The pseudogap influence on the BCS–BEC crossover

The possibility of a BCS–BEC crossover, namely an interpolation between weak and strong attractive interaction between the electrons, can be treated if we solve self–consistently equations (3) and (6). In the weak coupling limit (BCS case), the value of the chemical potential is fixed at the Fermi level, a self-consistent treatment of equations (3) and (6) being irrelevant. However, things are completely different in the strong coupling limit (BEC case), were due to a strong interaction between the electrons we expect a dramatic change in their chemical potential, and accordingly the two equations have to be considered at the same time. In the following we will discuss the solutions of the two coupled equations (3) and (6), and possible effects due to the pseudogap presence on the physical properties of HTSC as they result from these solutions.

The superconducting gap, Δ_0, as it results from equations (3) and (6) is plotted in Figure 1a as function of the pseudogap value, E_g, for different values of the system density. As the pseudogap value increases the superconductivity gap decreases, the superconducting phase being destroyed, a result which was already reported in reference [18]. For $E_g = 0$, the gap equation (3) reduces to the standard BCS gap equation. For the BCS case the gap equation has a real solution for any value of the attractive interaction V, the presence of the superconducting state being signaled by a nonzero value for the superconducting order parameter Δ_0. When the self-consistent problem is solved in the presence of a pseudogap, a critical attractive interaction is required for the existence of a superconducting state. Figure 1b presents the superconducting gap parameter Δ_0 as function of the attractive interaction V for different values of the pseudogap parameter E_g. The plot clearly identify a critical value for the interaction required for a nonzero value of the gap parameter. Moreover, the critical interaction value can be extracted as it follows. Let us consider the limit situation in which $\Delta_0 \to 0$. In such circumstances, equation (3) becomes

$$\frac{1}{V_{cr}} = \frac{1}{8\pi^2} \int_0^\pi dk_x \int_0^\pi dk_y \frac{\phi^2\left(\vec{k}\right) E_g^2 + 2\,E^2\left(\vec{k}\right)}{\left[\phi^2\left(\vec{k}\right) E_g^2 + E^2\left(\vec{k}\right)\right]^{\frac{3}{2}}}, \quad (7)$$

where $E(\vec{k}) = \epsilon(\vec{k}) - \mu$. Figure 2a presents results for the critical interaction V_{cr} as function of the pseudogap parameter E_g for different values of the system density. The results were obtained using a self-consistent calculation which involves both equation (7) and the density equation (6). In the weak coupling case, when the chemical potential is fixed at the Fermi level the density equation becomes irrelevant, and the value of the critical interaction V_{cr} can be obtained analytically. The corresponding solutions has the form $1/V_{cr} = (m/4\pi) \ln\left[0.892\,W/(E_g)\right]$, with W being a cutoff such that $W \gg E_g$. It is clear at this point that for $E_g \to 0$, $V_{cr} \to 0$, which means that in the absence of a pseudogap the superconducting state exists no matter how small the attractive electron-electron

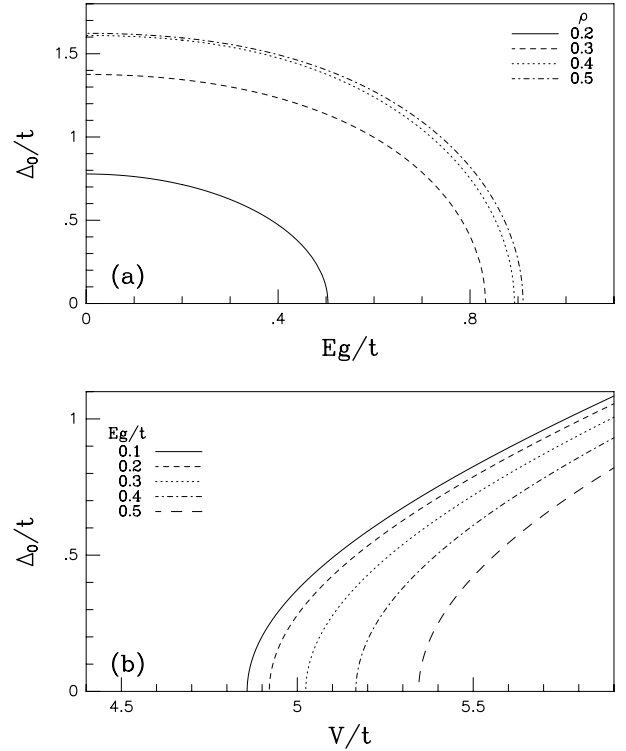**Fig. 1.** (a) The superconducting gap Δ_0/t as function of the pseudogap parameter E_g/t at different density values. (b) The superconducting gap Δ_0/t as function of the interaction strength for different values of E_g/t at a fixed density $\rho = 0.2$. (For both figures a d-wave model including next nearest neighbors hopping was considered ($\alpha' = 0.2$)).

interaction is. However, the presence of a pseudogap requires a critical interaction for a nonzero superconducting gap, meaning that if $V < V_{cr}$ a metallic–like state will be present in the HTSC phase diagram in the weak coupling regime.

Figure 2b presents the chemical potential as function of the attractive interaction strength V for different values of the pseudogap parameter E_g. The horizontal line at $\mu/t = -3.2$ represents the bottom of the tight-binding band. It is well know that in the weak coupling regime, the fermionic nature of the electronic system is conserved despite the fact that electrons form pairs. Such a behavior of the system is signaled by a value of the chemical potential above the bottom of the tight-binding band, equivalent with a positive chemical potential for the continuous model. On the other hand, in the strong coupling regime, at high attractive interactions, the value of the chemical potential for all curves is situated bellow this minimum of the tight-binding band, the system manifesting bosonic–like degrees of freedom. In this limit the attraction leads to small sized electronic pairs which behave like composite bosons able to undergo a BEC. The situation becomes much more complicated in the intermediate interaction regime, were the system should be described by a crossover theory which interpolates between the standard BCS and BEC pictures.
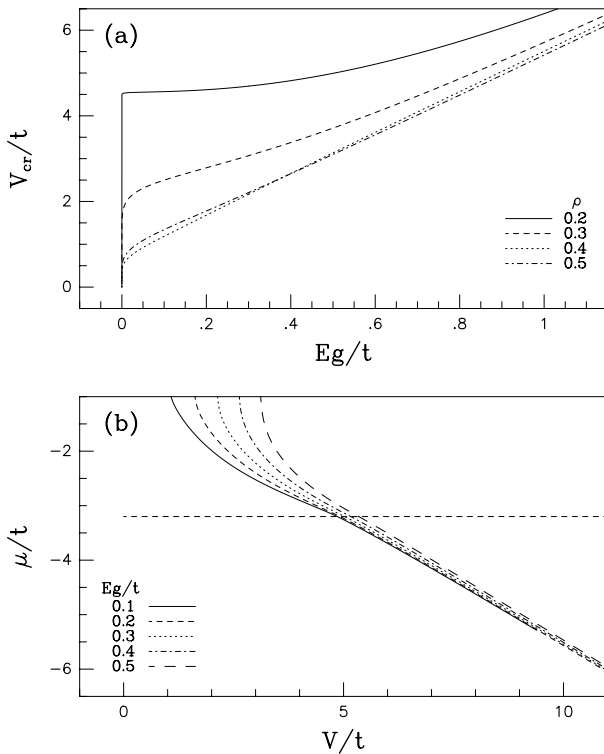
Fig. 2. (a) The required critical interaction V_{cr} as function of the pseudogap parameter value E_g at different density values. (b) The chemical potential as function of the interaction strength V for different values of the pseudogap parameter E_g. The dashed horizontal line represents the minimum of the conduction band, values for the chemical potential below this line being a signal of bosonic-like degrees of freedom. (For both figures a d-wave model including next nearest neighbors interactions was considered ($\alpha' = 0.2$).)

Fig. 3. (a) Possible phase diagram (ρ vs. $\log(V/t)$) for a d-wave superconductor for different values of E_g. Metallic-like ($\Delta_0/t = 0$), BCS-like, and BE-like phases are properly identified. (b) A better insight of the differences induced by different values of the pseudogap E_g. For both figures a d-wave model including next nearest neighbors interactions was considered ($\alpha' = 0.2$).

The density–interaction $T = 0$ K phase diagram of the HTSC usually consists in two different regions, associated to fermionic and bosonic degrees of freedom, respectively [19]. For the case of a system with s-wave symmetry of the superconducting order parameter, it was proved that a crossover between fermionic and bosonic degrees of freedom is possible at any values of the system density [14]. On the other hand, the situation for the case of a d-wave symmetry of the superconducting order parameter is much more controversial. den Hertog [20] and Soares et al. [21] claim that a non-pairing region, metallic–like phase, is present in the phase diagram at low attractive interactions. However, such a claim is in contradiction with the standard d-wave solution of the weak coupling BCS equation, which proves for the continuous model the existence of a superconducting state regardless the value of the attractive interaction between the electrons [22].

Figure 3 presents the effects of the pseudogap parameter E_g on the density–interaction phase diagram of the HTSC at $T = 0$. As we previously discussed, the consequences of the pseudogap presence in the normal state of the HTSC are summarized by the need of a critical attractive interaction in order to form pairs which will be subject of a BCS or BEC–like phase. Figure 3a presents a possible
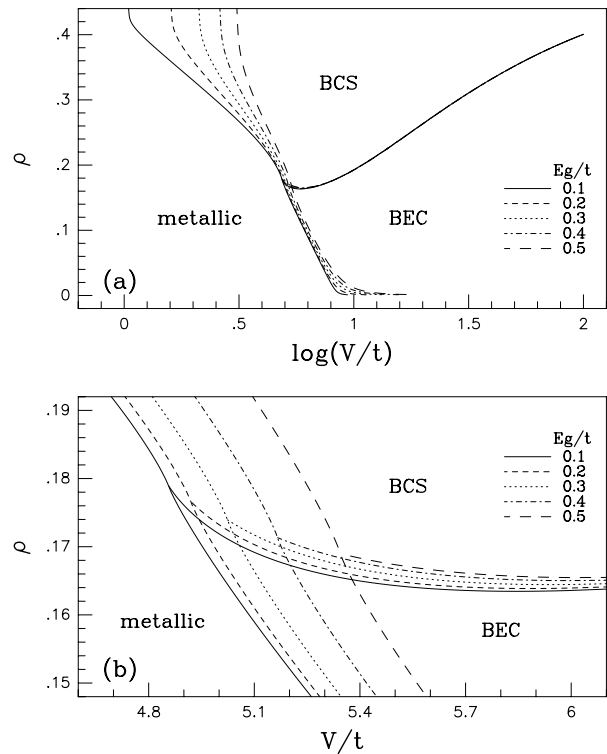
phase diagram for HTSC materials at different values of the pseudogap parameter E_g. In the weak coupling limit, when the interaction between the constituent electrons is small ($V < V_{cr}$), a metallic–like state is present. Such a state is identified by the condition $\Delta_0 = 0$, i.e., a superconducting state is absent. However, calling this state metallic, may be very inappropriate, as the presence of the pseudogap will have a strong effect on the system properties, meaning that the standard Landau theory of metals may not work in this situation. In the strong coupling regime ($V > V_{cr}$), the attractive interaction between the constituent electrons may lead to the formation of electronic pairs which can form a BCS or BEC–like state. The difference between the two possible states is made by the value of the chemical potential, which at the border between the two phases equals the energy value of the minimum of the tight-binding band. As Figure 3 shows, bosonic–like degrees of freedom are possible only at small densities and high attractive interactions. This result is in agreement with previous calculations in the literature [6,7]. The behavior of the system looks similar for different nonzero values of the pseudogap parameter. For any value of the pseudogap E_g all three phases of the phase diagram, metallic, BCS, and BEC–like are present (see Fig. 3b). The phase diagram was obtained considering only direct interactions

between the constituent electrons of the system. Once the electronic pairs are formed, especially in the strong coupling limit, there is a possibility that pair–pair interaction will be relevant to the problem, approximations beyond the usual mean–field treatment being required [23].

4 Conclusions

In conclusion we have obtained the phase diagram of a HTSC at $T = 0$ K in the case of a d-wave symmetry of the order parameter. The role of the pseudogap parameter E_g on the phase diagram was considered in a phenomenological way, by introducing its effects as corrections to the free electron state via an additional term in the self-energy. The form of such a term can be justified by the analysis of the experimental data obtained from ARPES measurements [5]. Our calculations, both analytical and numerical, proved that the pseudogap effects can be drastic on the density–interaction phase diagram of HTSC, a metallic–like state being identified in the weak coupling regime. The question that this state is pure metallic, or is of a different nature, is still open, further calculations being underway. Our calculations should be relevant for the underdoped cuprates, where the presence of the pseudogap was experimentally proved. However, if the presence of the pseudogap will be proved also in the overdoped region of the HTSC temperature–doping phase diagram the calculations presented here will correctly describe this region of the phase diagram too.

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